

Butanoic anhydride
106-31-0 | DTXSID8026729

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.68e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.16e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

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Ethyl heptanoate

Measured: 2.83e-01

Predicted: 9.64e-01

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Ethyl valerate

Measured: 2.08e-01

Predicted: 4.56

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2,4-Pentanedione

Measured: 1.36

Predicted: 3.07

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1,3-Diethylbenzene

Measured: 7.80e-01

Predicted: 9.75e-01

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N-Methylcarbamic acid, ethyl ester

Measured: 8.92e-01

Predicted: 1.51